



## A TAU METHOD BASED ON NON-UNIFORM SPACE-TIME ELEMENTS FOR THE NUMERICAL SIMULATION OF SOLITONS

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**Abstract**—In this paper we discuss the numerical simulation of soliton solutions of Schrödinger's system of nonlinear partial differential equations. The technique used is based on a novel approach to the Tau Method based on *space-time elements*. The original operator is not discretized in either space or time. The perturbation term, which in the Tau Method is a by-product of the computation, is used to measure the error in the equation, or *defect*, and therefore to control the accuracy of the computation in an adaptive way. This leads to an accurate and economical numerical procedure which, even for approximations of a very low degree, can simulate surfaces with very sharp gradients in the direction of both, space and time.

The Tau Method formulation presented in this paper preserves very accurately the principle of conservation of energy. However, our numerical examples support the idea that the latter is a necessary but not a sufficient condition to guarantee an efficient approximation of soliton solutions of Schrödinger's equation by means of a method of numerical simulation.

### 1. INTRODUCTION

In recent years several authors have reported results of experiments on the numerical solution of Schrödinger's nonlinear partial differential equation in one space dimension [1-8]. Approximate solutions to this equation and to others of related type, such as the Korteweg-de Vries equation and the sine-Gordon equation, are of interest in view of their relevance to problems in Physics and in advanced Engineering design. They are also of interest from a purely numerical standpoint because of the nature of their solutions, which display high gradients in their domain of definition.

A substantial part of such numerical work has been carried out using sophisticated discrete variable techniques although Galerkin's method has also been used. The approach considered in this paper is a global one based on the Tau Method [9-10] and does not involve discretization of the differential operator in the space or time directions.

In the case of a *linear* problem a Tau approximate solution takes the form of a bivariate polynomial which satisfies exactly a differential equation identical to the given one but with a polynomial term, which we shall indicate with  $H_{NM}$ , appended to the right hand side. The role of this perturbation term is to reduce the solution, generally a bivariate function, to a bivariate *polynomial*. There is also the requirement that the *norm* of this extra term satisfies a minimum condition, so that the deviation from the original equation, that is, the error in the equation, is as small as possible. The latter, often called *defect* in the context of finite difference techniques, is immediately accessible to the user in the Tau Method and used to monitor the progress of the computation.

In the case of a *nonlinear* problem the Tau Method is used to solve iteratively a series of interrelated linear problems. Their solution generates a sequence of polynomials; its fixed point is the required Tau Method approximate solution of the given nonlinear problem. In the case

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of the Tau Method such a process has been described in a series of papers by Ortiz [11], Ortiz and Samara [12], Ortiz and Pham Ngoc [13] and Onumanyi and Ortiz [14] for the case of initial, boundary and multipoint problems for *ordinary* differential equations and in Ortiz and Samara [15], Ortiz and Pun [16] and Ortiz and Pham Ngoc [17] for the case of *partial* differential equations and in further references given therein.

In a recent paper published in this *Journal*, Ortiz and Pun [18] discussed the application of a segmented formulation of the Tau Method, introduced by Ortiz [19], to the numerical solution of nonlinear partial differential equations; there the domain is subdivided into small cells. They have applied this approach to the numerical treatment of Burgers' nonlinear partial differential equation reporting results of high accuracy and smoothness. Numerical comparisons with standard software, such as the efficient code of Sincovec and Madsen [20] indicate that the Tau Method can be an interesting alternative from the point of view of efficiency as well as on account of its accuracy.

In several of the papers to which we referred earlier on, more particularly in those of Griffiths, Mitchell and Morris [2], Herbst, Morris and Mitchell [4] and Verwer and Sanz-Serna [8], a series of interesting numerical examples are considered. Some of these examples will be reconsidered in this paper using the Tau Method with uniform and non-uniform *space-time* Tau elements.

## 2. SCHRÖDINGER'S CUBIC EQUATION

Let us consider Schrödinger's cubic equation

$$i u_t + u_{xx} + q |u|^2 u = 0, \quad (1)$$

on a space-time domain  $\Gamma$ , where  $i^2 = -1$ , with the initial condition

$$u(x, 0) := g(x), \quad -\infty < x < \infty, \text{ and } t \geq 0. \quad (2)$$

As the solution of this problem is a complex valued function,  $u(x, t) := v(x, t) + i w(x, t)$ , we shall regard it as implicitly defined by a *system* of nonlinear partial differential equations. The solution of problem (1)–(2) has an infinite set of conservation laws [21] one of which is the *conservation of energy* in time, that is, of

$$E(u) = \int_{-\infty}^{\infty} |u(x, t)|^2 dx, \quad \text{for } t > 0.$$

This condition states the boundedness of the norm of the solution in the space  $L^2[-\infty, +\infty]$  and is a necessary condition to keep the balance between the nonlinear term  $|u|^2 u$  and the dispersive  $u_{xx}$  term in the equation. When such balance occurs, solitons are formed (for further details, see [22–24]).

We shall consider cases where either particular values of the nonlinear parameter  $q$  or given particular initial conditions determine the emergence of solitons. The problems to be considered are:

- (i) the case of one soliton,
- (ii) the collision of two solitons, and
- (iii) bound states of  $N$  solitons.

The first case, where the analytic solution is known, enables us to show that the remarkable accuracy associated with the segmented formulation of the Tau Method in the numerical treatment of ordinary differential equations with spikes (see Onumanyi and Ortiz [14]) is also present in the case of the system of nonlinear partial differential equations considered here. We also show that the energy dependent parameter  $E(u)$  is very accurately conserved by the Tau Method approximate solution as time advances.

### 3. CONSTRUCTION OF THE TAU APPROXIMATE SOLUTION: SPACE-TIME TAU ELEMENTS

Let us associate with equation (1) the recursive scheme defined by:

$$\begin{aligned} v_{xx}^{[n+1]} - w_i^{[n+1]} + 2qv^{[n]}w^{[n]}w^{[n+1]} + q[3(v^{[n]})^2 + (w^{[n]})^2]v^{[n+1]} &= 2qv^{[n]}[(v^{[n]})^2 + (w^{[n]})^2], \\ w_{xx}^{[n+1]} + v_i^{[n+1]} + 2qv^{[n]}v^{[n+1]}w^{[n]} + q[3(w^{[n]})^2 + (v^{[n]})^2]w^{[n+1]} &= 2qw^{[n]}[(w^{[n]})^2 + (v^{[n]})^2] \end{aligned} \quad (3)$$

on  $\Gamma$ , which follows from (1) bearing in mind that  $u(x, y)$  is a complex valued function and after applying a quadratic linearization process (see [17] and the references given therein).

The initial condition (2) becomes:

$$v^{[n]}(x, 0) = \text{Real}[g(x)] \quad \text{and} \quad w^{[n]}(x, 0) = \text{Imag}[g(x)]. \quad (4)$$

For each value of  $n$  scheme (3) defines a system of *linear* partial differential equations with variable (bivariate polynomial) coefficients, to which the Tau Method is immediately applicable, as it is shown in [15].

We shall indicate by  $u_{MN}(x, t)$  a Tau approximation of degree  $M$  in  $x$  and  $N$  in  $t$ . Convergence of the sequence of approximations  $u^{[n]} := (v^{[n]}, w^{[n]})$ ,  $n = 0, 1, 2, \dots$  will be monitored by comparing the corresponding coefficients of successive iterates. The approximation process is stopped when the maximum of these differences falls below a prescribed tolerance parameter  $TOL$ . This comparison shall be made in an orthogonal polynomial basis, where the coefficients in the expression for  $u_{MN}$  become stable much faster than in a representation in terms of powers of the variables.

The solutions  $u$  of (1)–(2) are characterized by the fact that, for  $t \in [0, T]$ ,  $|u|$  is very small outside an interval  $x_L \leq x \leq x_R$ . We shall make use of this feature in our numerical computation by solving the problem in that interval of  $x$ , with the initial condition  $u(x, 0) = g(x)$  and assuming  $u_x = 0$  when  $x = x_L$  and  $x = x_R$ , for values of  $t$  in the interval  $0 \leq t < T$ . This argument has been used by several other authors who considered this problem before us (see [2, 4] and the references given therein). Therefore, throughout this paper we shall consider a domain  $\Gamma$  as defined by  $[x_L, x_R] \times [0, T]$ .

We shall partition  $\Gamma$  into subdomains, which we call *space-time Tau elements* [18]; they have sides  $h_x$  and  $h_t$  parallel to the axis. Let  $ij$  be a pair of indices which identifies each one of the cells and let  $M$  and  $N$  be the degrees of approximation in  $x$  and  $t$  respectively. Our numerical task is to solve system (3)–(4) iteratively over each of the cells of indices  $ij$ , which are intercommunicated by suitable continuity conditions. Inside each these cells we solve the system of partial differential equations defined by (3) with the Tau Method to get individual bivariate polynomials  $u_{MNij}^{[n]}(x, t)$  associated with each cell at each stage  $n$  of the iterative process.

It has been shown that the accuracy of a one-dimensional Tau Method approximate solution at the end point of the approximation range depends closely on the basis used for the representation of the perturbation term [25–26]. Theoretical results giving quantitative estimates for a wide range of choices of basis have been discussed by Namasivayam and Ortiz in [27]. The same arguments apply for the *edges of a bi-dimensional Tau cell*. In the problems considered here, where information is transmitted through the boundaries of a large number of space-time Tau Elements, taking such effect into account has some relevance. We shall come back to this question later, when he discusses the relative efficiency of Chebyshev and Legendre bases for the representation of the perturbation term  $H_{MN}(x, t)$ .

### 4. THE CASE OF ONE SOLITON

With the initial condition

$$u(x, 0) := g(x) = (2\alpha)^{\frac{1}{2}} \exp \left[ i \left( \frac{cx}{2} \right) \right] \text{sech} (\alpha^{\frac{1}{2}} x), \quad (5)$$

and  $q = 1$ ; Equation (1) allows for the emergence of one soliton which propagates in the direction of time. The parameters  $\alpha$  and  $c$  are positive constants.

Table 1. Approximation error and energy conservation in the case of one soliton.

A bicubic Tau Method approximation on Tau Elements of size $h_x \times h_t$ was used					
$h_x$	$h_t$	basis	max. abs. error		
			$t = 0$	$t = 15$	$t = 30$
0.5	0.25	Chebyshev	0.1451	0.2711	0.3949
			3.9998	3.9998	3.9998
0.5	0.125	Chebyshev	0.0531	0.1860	0.3128
			3.9998	3.9998	3.9998
0.5	0.25	Legendre	0.1380	0.1457	0.1538
			4.0000	4.0000	4.0000
0.5	0.125	Legendre	0.0494	0.0577	0.0659
			4.0000	4.0000	4.0000
0.25	0.125	Legendre	0.0442	0.0447	
			4.0000	4.0000	4.0000

The analytic solution of Equation (1) is known to be [22]

$$u(x, t) := (2\alpha)^{\frac{1}{2}} \exp \left\{ i \left[ \left( \frac{cx}{2} \right) - \left( \frac{c^2}{4 - \alpha} \right) t \right] \operatorname{sech} \left[ \alpha^{\frac{1}{2}} (x - ct) \right] \right\}, \quad (6)$$

Verwer and Sanz-Serna computed estimates of the solution of this problem for  $\alpha = 1$  and  $c = 1$  in [8].

We shall use the artificial boundary conditions  $u_x = 0$  at  $x = x_L$  and  $x = x_R$ , with the choices:  $x_L := -30$  and  $x_R := 70$ . From (5) it follows that the maximum of  $|u(x, 0)| = 2^{\frac{1}{2}}$ ; in the above case

$$E(u) = \int_{-30}^{70} |u(x, 0)|^2 dx = 4. \quad (7)$$

Let us compare the relative efficiency of using Chebyshev or Legendre bases in the numerical approximation of this problem. That is, the effect of ignoring or not the increased accuracy at matching edges of cells which is provided by the last basis. In Table 1 we give, for  $t = 0, 15$  and  $30$ , the maximum absolute error (in the top row) obtained by using Tau approximations of degree 3 in each of the two variables and for several different sizes of Tau cells, in either the Chebyshev or the Legendre basis. We use the value of  $E(u)$  given by (7) as a reference and report on estimates for it obtained by computing the quantity  $E(u_{MN})$  (in the lower row).

Replacement of the Chebyshev basis of representation by that of Legendre ( $h_x = 0.5$  and  $h_t = 0.25$  or  $h_t = 0.125$ ) produces a sensible reduction in the approximation error for large values of  $t$ . Energy is well conserved by using any of the two basis.

It has been pointed out [28] that numerical estimations of the soliton solution of (1) develop a *shift in time* if compared with the analytic solution. Figures 1A–1F show the graphs of  $|u| = [v^2 + w^2]^{1/2}$  for the exact and also for the Tau approximate solution for different choices of the parameters and for the two bases mentioned before. Graphs A and B show that in the Chebyshev bases a reduction to a 1/2 of the length of the side  $h_t$  of the cell has a positive effect in reducing the shift at  $t = 30$ . However, a similar but more dramatic effect is obtained by changing into the Legendre basis, as shown by graphs C and D. Finally, graphs E and F display the behaviour of the exact and approximate curves for  $t = 15$  in the Legendre basis. The improved accuracy provided by the Legendre basis at the edges of matching space-time Tau cells seems to have a bearing on the reduction of the shift phenomenon.

The curves in Figure 2 show the graphs of  $|u_{33}|$ , the bicubic Tau Method approximate soliton solution, in the time range  $[0, 30]$  for  $0(1.5)30$ , that is, at intervals equal to 1.5. Graphs correspond to the choice of space-time Tau elements with  $h_x := 0.5$  and  $h_t := 0.125$ ; on account of the previous remarks, the Legendre basis has been used.

MOD. U FOR T=0. AND T=30.

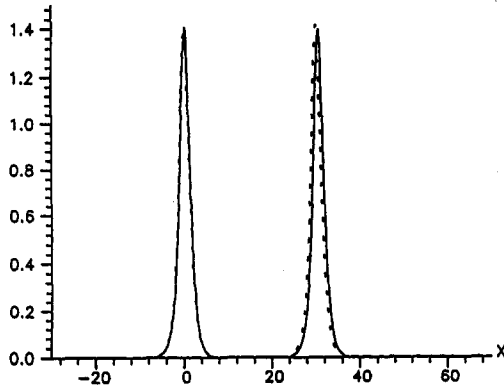


Figure 1A.  $h_x := 0.5$ ,  $h_t := 0.25$ ,  
 $t := 30$ , Chebyshev basis;

MOD. U FOR T=0. AND T=30.

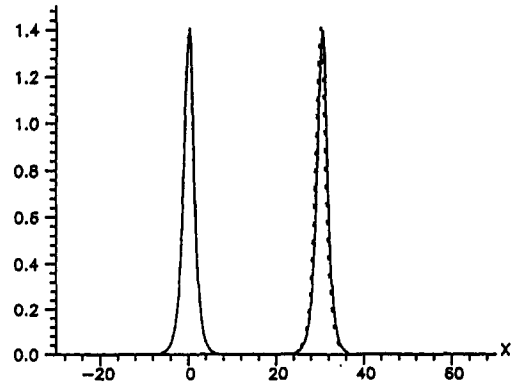


Figure 1B.  $h_x := 0.5$ ,  $h_t := 0.125$ ,  
 $t := 30$ , Chebyshev basis;

MOD. U FOR T=0. AND T=30.

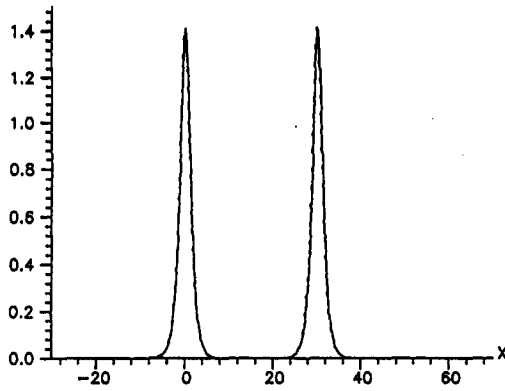


Figure 1C.  $h_x := 0.5$ ,  $h_t := 0.25$ ,  
 $t := 30$ , Legendre basis;

MOD. U FOR T=0. AND T=30.

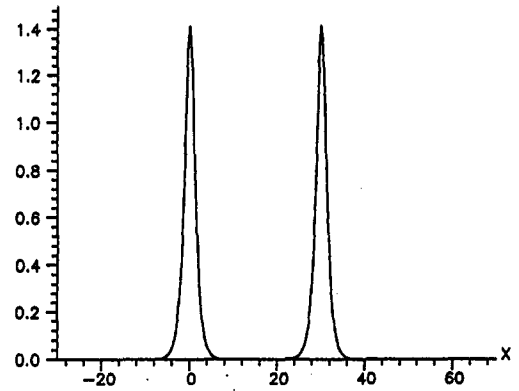


Figure 1D.  $h_x := 0.5$ ,  $h_t := 0.125$ ,  
 $t := 30$ , Legendre basis;

MOD. U FOR T=0. AND T=15.

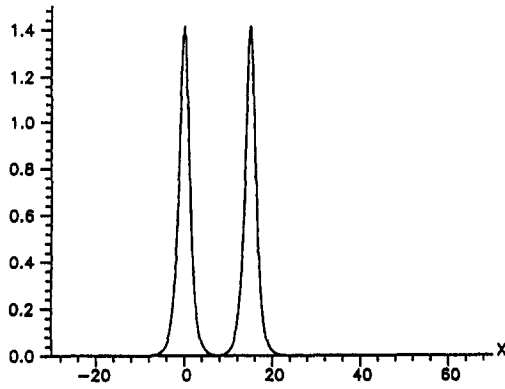


Figure 1E.  $h_x := 0.5$ ,  $h_t := 0.125$ ,  
 $t := 15$ , Legendre basis;

MOD. U FOR T=0. AND T=15.

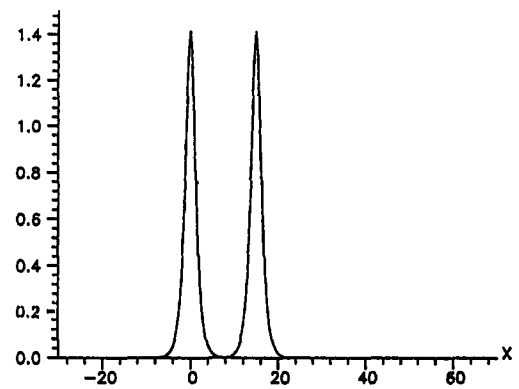


Figure 1F.  $h_x := 0.25$ ,  $h_t := 0.125$ ,  
 $t := 15$ , Legendre basis.

Figure 1. Graphs showing the shift in time between the exact solution, in dotted curve, and the Tau approximate solution, in solid curve, for  $t = 0$ ,  $t = 15$ , or  $t = 30$  in Chebyshev or Legendre bases for the different sizes of Tau-Elements.

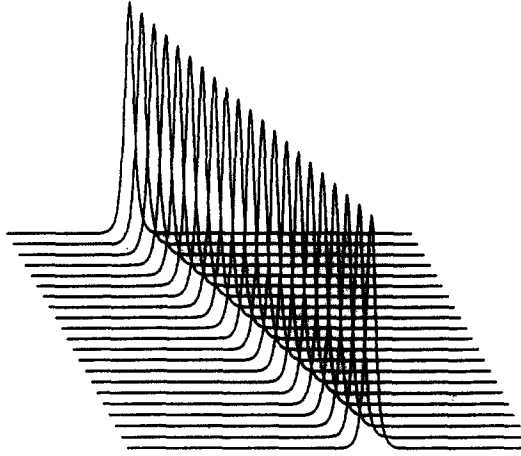


Figure 2.  $|u_{33}(x, t)| = [(v_{33}(x, t))^2 + (w_{33}(x, t))^2]^{1/2}$ , bicubic Tau approximation in the Legendre basis over the domain  $[-30, 70] \times [0, 30]$ . Individual graphs correspond to  $t = 0(1.5)30$ ; the size of the Tau Elements is  $0.5 \times 0.125$ .

The graphs of the Tau approximations are remarkably smooth. On each time line the maximum absolute error reaches a peak at the points where the spike of the soliton wave is located.

The relative error defined by the perturbation term  $H_{MN}$  through

$$\Psi_{33} = \max \left\{ \frac{|H_{33}(x, t)|}{\max |u_{33}(x, t)|} \right\}$$

over the domain  $\Gamma := [-30, 70] \times [0, 30]$ , follows the same pattern and reaches the value  $0.37/1.4 = 0.26$  at the points of  $\Gamma$  corresponding to the position of the maxima; however, the approximation error at that point remains small, in the order of  $10^{-2}$ .

## 5. COLLISION OF TWO SOLITONS

Let us again consider the cubic Schrödinger's equation (1), but now with the initial condition:

$$g(x) := \left( \frac{2\alpha}{q} \right)^{\frac{1}{2}} \left[ \exp \left( \frac{ic_1 x}{2} \right) \operatorname{sech} (x\alpha^{\frac{1}{2}}) + \exp \left( \frac{ic_2(x - \delta)}{2} \right) \operatorname{sech} (\alpha^{\frac{1}{2}}(x - \delta)) \right]. \quad (8)$$

We shall take  $\alpha := 0.5$ ,  $q := 1$  and  $c_1 := 1$  for the fastest soliton and  $c_2 := 0.1$  for the slower one. The parameter  $\delta$  controls the relative location of the solitons at the origin of time; we take  $\delta := 25$ .

We have considered a fairly large domain  $\Gamma := [x_L, x_R] \times [0, T]$ , where  $x_L := -20$ ,  $x_R := 80$  and  $T := 44$  and have initially covered it with equal Tau elements of sides  $h_x = h_t := 0.25$ . After 176 rows of cells in time we reach the end of our domain. Again, we have chosen bicubic Tau approximations in each element.

Figure 3 shows separate graphs of the two solitons at  $t = 0$  and then from  $t = 18$ , when they start to interact, until  $t = 30$ , when they begin to disengage. We have taken subintervals of length 2 in time. The graphs for  $t = 22$  and 24 show clearly that the interaction is not a simple superposition. Successive graphs on a time scale  $0 \leq t \leq 44$  are displayed in Figure 4. After collision the path of each of the solitons develops a *phase shift* which, for one of them, is indicated in Figure 4 with two parallel arrows: they point at the directions before and after collision.

The same sequence of graphs, now superimposed to show more clearly the behaviour near the collision point, is shown in Figure 5. The calculation was repeated with a Tau approximation of the same order, but with the length of  $h_t$  halved. In Figure 6 results are shown, with the same format as in Figure 5, where we have only displayed graphs up to  $t = 30$ , just after the collision point.

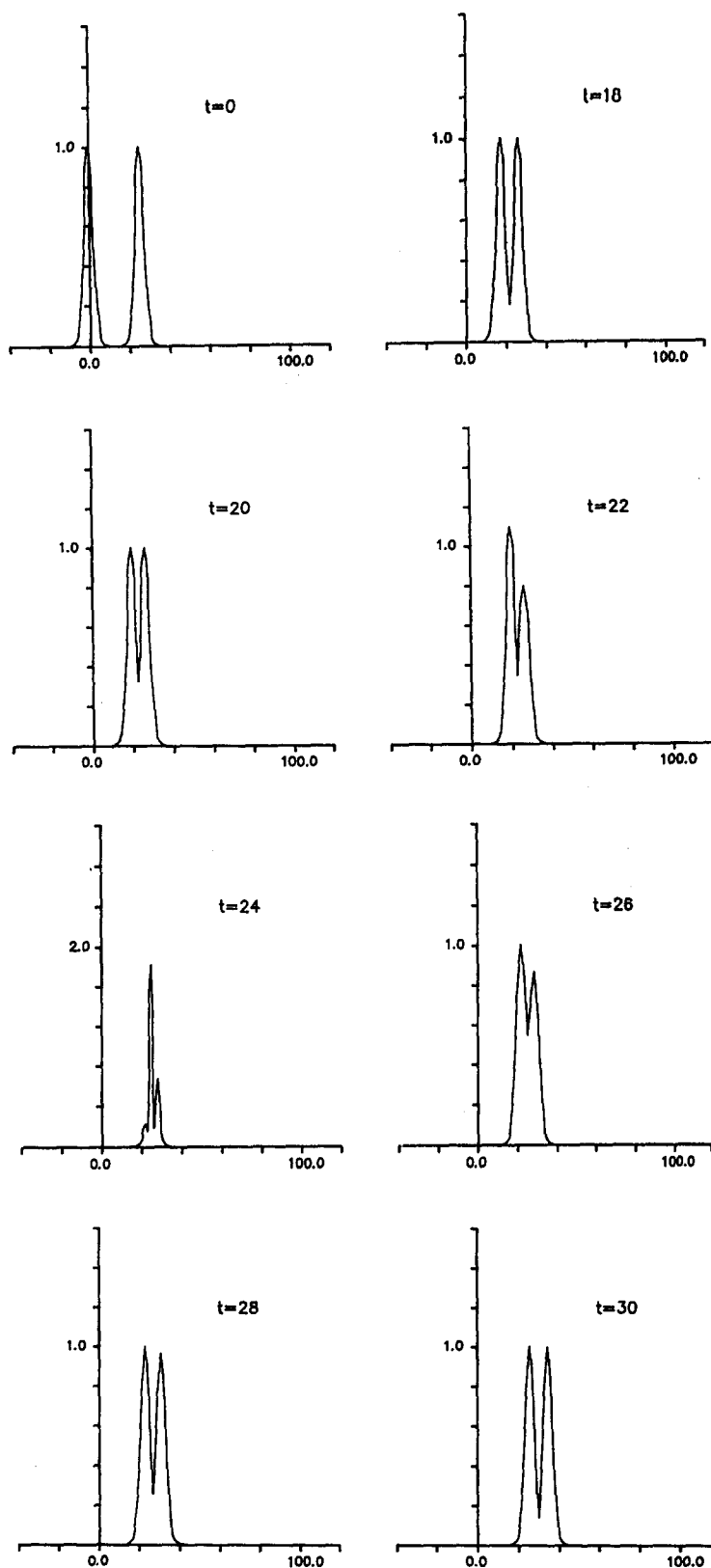


Figure 3. Individual graphs of a Tau Method approximation to the two-soliton solution corresponding to the initial condition (8), at  $t = 0$  and  $t = 18(2)30$ .

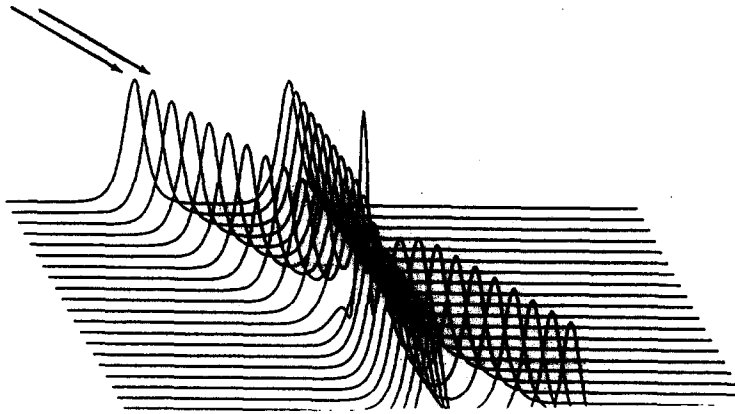


Figure 4. The same problem as in Figure 3: graphs displayed on a time scale,  $t = 0(2)50$ ;  $h_x = h_t := 0.25$ . The two parallel arrows on the top left show the shift in phase of one of the solitons; the shift in phase of the other soliton is not marked but is visible in this figure.

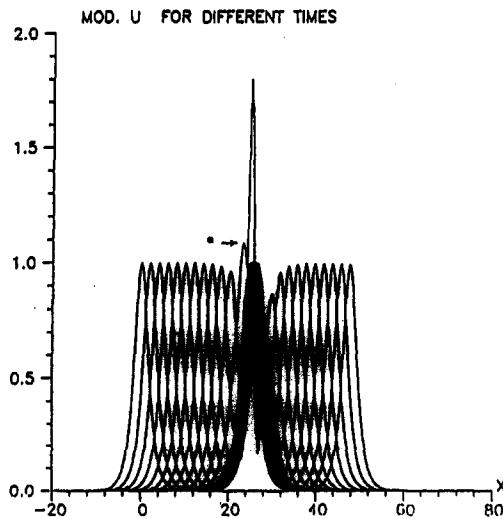


Figure 5. The same problem as in Figure 4: a sequence of superimposed graphs for  $t = 0(2)50$ ;  $h_x = h_t := -0.25$ .

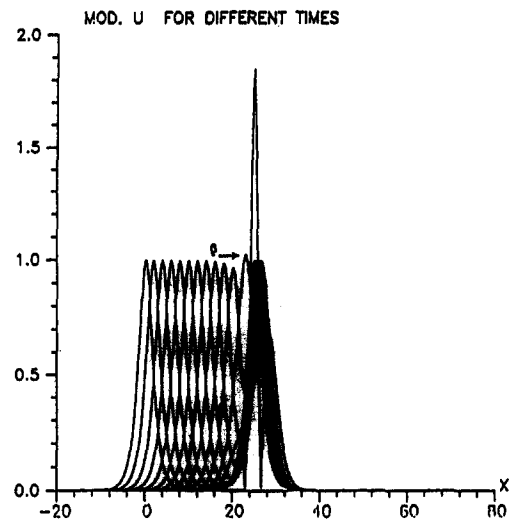


Figure 6. The same problem as in Figure 5: a sequence of superimposed graphs for  $t = 0(2)30$ ; now with  $h_x := 0.25$ ,  $h_t := 0.125$ .

Comparing Figure 6 with Figure 5 we notice that the distortion before the collision (for  $t = 22$ , pointed by arrows  $\beta$  and  $\alpha$  respectively) has been reduced in amplitude. Later we shall refer to the curve pointed by the arrow  $\beta$  as the *lower curve*.

In the present case we cannot offer comparisons with a known analytic solution. However, in Figure 7 we show the behaviour of the modulus of the error in the equation for this Tau problem, that is, of the perturbation term  $H_{33}(x, t)$ , for different values of  $t$ .

The first of them, Figure 7A, corresponds to a calculation with  $h_x = h_t := 0.25$ . It has been plotted for a range that includes  $t = 0(2)44$  and shows that the error in the equation becomes larger in a small interval around the collision point, as is to be expected due to the very rapid rise of  $|u|$  near it. Figure 7B shows the effect on the error caused by reducing the length of  $h_t$  to half of its previous value, while keeping  $h_x := 0.25$  as before;  $t$  has been taken again in a range that includes  $0(2)50$ . The error pattern is similar, but reduced in amplitude.

In particular, the error just before the collision is also reduced in the second case, as compared with the first. This suggests that the  $\beta$ -arrowed *lower curve* in Figure 6, for  $t = 22$ , which shows a less accentuated peak before collision than the corresponding one in Figure 5, may offer a better picture of the collision of the two solitons.



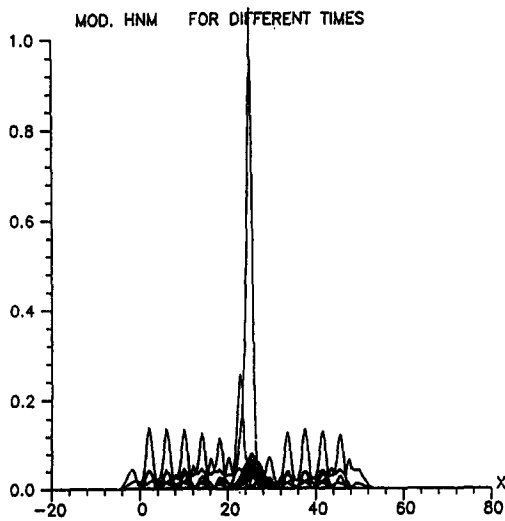
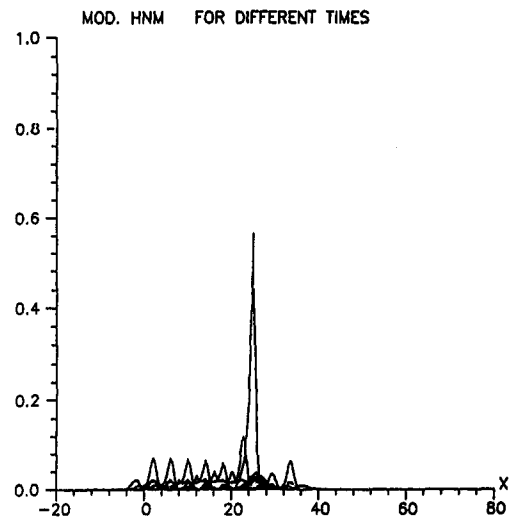
Figure 7A.  $h_x = h_t := 0.25; t = 0(2)44$ Figure 7B.  $h_x := 0.25; h_t := 0.125; t = 0(2)44$ .Figure 7. Graph of the modulus of the perturbation term  $H_{33}(x, t)$ .

Table 2. Behaviour of the maximum modulus of the perturbation term in the collision of two solitons.

Max $ H_{33}(x, t) $ for different values of $t < T$ and $-20 \leq x \leq 80$ ; a bicubic Tau Method approximation on Tau Elements of size $h_x \times h_t$ was used			
Problem	in the interval before the collision $0 \leq t \leq 20$	near the collision point $t = 24$	in the interval after the collision $26 \leq t \leq 44$
A	0.1390	1.065	0.1391
B	0.0722	0.565	0.0674
C	0.1625	1.2493	0.1616

Problem A.  $h_x := 0.25; h_t := 0.25$  Chebyshev basis  $T := 0(2)44$ ;Problem B.  $h_x := 0.25; h_t := 0.125$  Chebyshev basis  $T := 0(2)44$ ;Problem C.  $h_x := 0.5; h_t := 0.25$  Legendre basis  $T := 0(2)44$ .

Table 2 gives quantitative information on the effect of changing the basis of representation for the perturbation term. A comparison of the second and last entries, shows that for this bicubic Tau approximation a Legendre basis with space length equal to  $h_x := 0.5$  (problem C) gives about the same value for the maximum modulus of the perturbation term (defect error) as a Chebyshev basis with sides of length equal to a half of the previous value:  $h_x := 0.25$  (Problem A).

## 6. CONSERVATION OF ENERGY IN THE TAU METHOD

Another way of testing the behaviour of a Tau Method approximate solution is by checking the energy dependent parameter  $E(u)$  for different values of  $t$  while  $x$  is in the interval  $-20 \leq x \leq 80$ . Making use of the initial condition we can estimate that  $E(u)$  to be equal to 5.65685... for  $t = 0$ . Evaluations of  $E(u_{33})$  for the same set of parameters and bases as in the Problems A, B and C considered before gave estimates agreeing with that reference value up to five significant figures. Finally, a comparison between Problems A and B in Table 2, shows that despite a dramatic change in  $\max |H_{33}(x, t)|$ , the energy remains unchanged and fixed within five significant figures.

This suggests that the conservation of energy is not sufficient to guarantee an accurate numerical approximation, other invariants may have to be considered. Our statement is in agreement with the experience of other authors, who used different numerical techniques. Although the energy condition should not be ignored, it must be borne in mind that conservation of energy alone can only ensure that the numerical solution lies on the surface of the sphere  $\rho = E(u)$ . By

generating a suitable artificial right hand side a numerical technique can be made to produce a spurious approximation which, nevertheless, remains on that surface.

In the case of the Tau Method we have the advantage that such a perturbation term, namely  $H_{mn}(x, t)$ , is at our disposal. We can then use it, when solving a nonlinear problem, to monitor the agreement of the approximate solution with the given differential equation at each step of the iterative process; such control has been used in our computations. Therefore, a truly adaptive process is feasible with Tau Method approximations (see [14] for more details).

A theoretical analysis of the convergence of the iterative process shows that it is fast (for analytic convergence results, see [17]). In the examples under discussion the number of iterations required to satisfy a tolerance parameter  $TOL$  equal to  $10^{-6}$  was only equal to 3 except at the collision point, where 4 iterations were required.

Griffiths, Mitchell and Morris [2] have reported estimates of  $E(u)$  for the initial value  $t = 0$  and for the final value  $t = 48.75$  using different sizes of  $t$  and  $x$ -meshes, running from 0.04167 to 0.125 in  $t$  and from 0.333 to 1.0 in  $x$  and using either Galerkin's method or finite difference techniques. Although it is clearly difficult to make comparisons with such very different approaches, it seems reasonable to state that the results reported by using a Tau Method approximation of a relatively low degree, 3 in  $x$  and 3 in  $y$ , seem to be associated with greater accuracy. This confirms experience gained by the authors in a variety of different problems for nonlinear systems of partial differential equations.

## 7. BOUND STATES OF MORE THAN ONE SOLITON: THE USE OF NON-UNIFORM SPACE-TIME TAU ELEMENTS

Herbst, Morris and Mitchell [3] and more recently Shamardan [29] considered a more difficult example, taking for the nonlinear parameter  $q$  in Schrödinger's equation (1) a much larger value:  $q := 18$ . The initial condition they selected was  $g(x) := 1/\cosh x$ , for  $t = 0$ .

This is a particularly interesting case, as the solution develops very steep spatial and temporal gradients. Since the solution is smooth outside the interval  $-10 \leq x \leq 10$ , we shall use here a *non-uniform covering* of the domain with Tau cells. We start with a very large  $h_x$ , which is later reduced, twice, as we approach the domain where the solution exhibits its largest variations. We have taken in our computations:

- (1)  $h_x := 5.0$  for  $20 \geq |x| \geq 10$ ;
- (2)  $h_x := 1.8$  for  $10 > |x| \geq 1$  and
- (3)  $h_x := 0.125$  for  $1 > |x|$ .

Thus, only 30 Tau Elements are required to cover the  $x$ -range. We have taken  $h_t := 0.01$  uniformly and solved for  $0 \leq t \leq 2.5$  using Tau approximations of degree 5 in each variable.

Figure 8 shows the graph of the absolute value of the Tau approximate solution  $u_{55}(x, t)$  in that domain. Figure 9 displays the surface  $v_{55}(x, t)$ , the real part of  $u_{55}(x, t)$ . Strong gradients in both the space and time directions are clearly visible in this graph. To check that all spikes are of the same height we have computed the absolute value of  $u_{55}$  at the points  $(0, t)$  from  $t = 0$  up to  $t = 2.5$ . This is shown in Figure 10, where the dots indicate the points of evaluation for different values of  $t$ . The Tau Method approximate solution surfaces given here have a far more neat and sharper shape than those reported by Shamardan [29] in his recent paper.

The degree of the Tau Method approximations was chosen to be equal to 5 in each variable, higher than before, on account of the severe variations of the solution and with the desire to keep the number of iterations very low. Although the tolerance parameter  $TOL$  was again fixed to be equal to  $10^{-6}$  only three iterations were sufficient to secure the convergence of the process except for  $|x| < 1$ , that is, near the spikes, where only *one* more iteration was required. The modulus of  $H_{55}(x, t)$  remained bounded by 0.16; a relative maximum is attained at the points corresponding to the position of the spikes of  $|u_{55}(x, t)|$  lie and it is much smaller, of the order of 0.04, away from them. Figure 11 shows the graph of  $|H_{55}(x, t)|$  for  $x = 0$  and for different values of  $t$ . The dots have the same meaning as before. The relative error  $\Psi_{55}$ , introduced earlier, and now defined over the domain  $\Gamma := [-20, 20] \times [0, 2.5]$  is, for this choice of  $M$  and  $N$ , considerably small: equal to  $0.16/2.4 = 0.06$ .

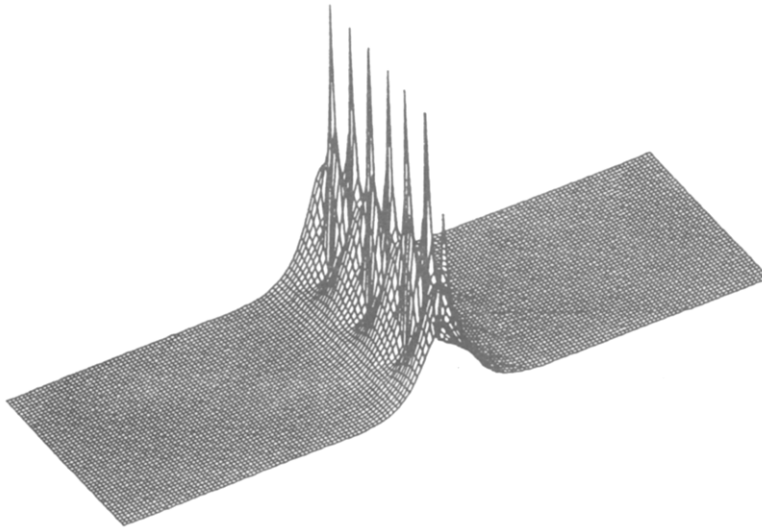


Figure 8. Graph of  $|u_{55}(x, t)| = [(v_{55}(x, t))^2 + (w_{55}(x, t))^2]^{1/2}$ , biquintic Tau approximation of  $u(x, t)$  over the domain  $[-20, 20] \times [0, 2.5]$ . The size of *space-time* Tau elements changes over different parts of the domain.

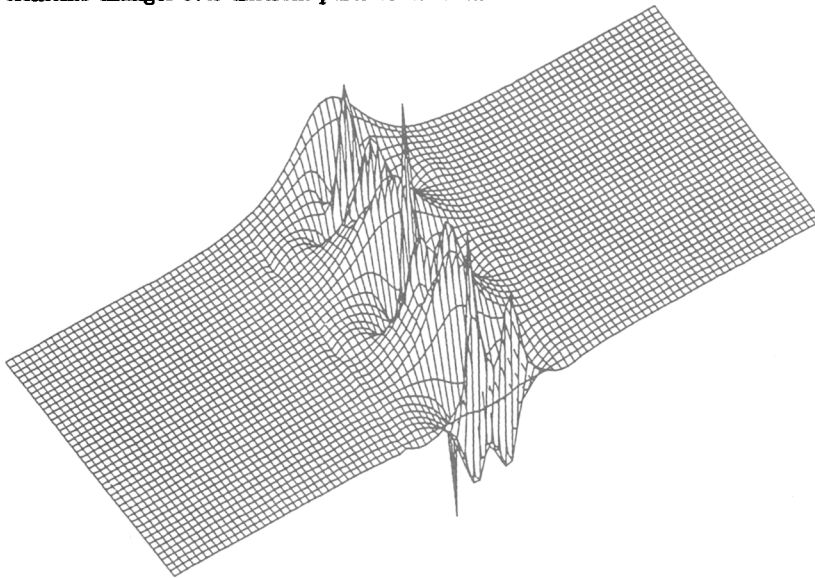


Figure 9. Graph of  $v_{55}(x, t)$ , the real part of  $u_{55}(x, t)$ .

## 8. FINAL REMARKS

It should be pointed out that the satisfaction of the tolerance parameter  $TOL$  and also of the conservation of energy are in no way sufficient conditions for the existence of an accurate numerical solution. It is possible to give examples of nonlinear partial differential equations where the first two conditions are satisfied while the numerical solution generates a large perturbation term  $H_{MN}$ . These last requirements must always be complemented, at least, by a check on the size of the perturbation term, that is, on the accuracy with which the equation is satisfied by the proposed approximate solution. This is a useful additional piece of information which the Tau Method gives with the approximate solution at no extra cost.

The application of the Tau Method to problems involving soliton interactions and, more generally, to systems of nonlinear partial differential equations in which the solution experiences large gradients in the direction of all variables, seems to be an area worthy of further research.

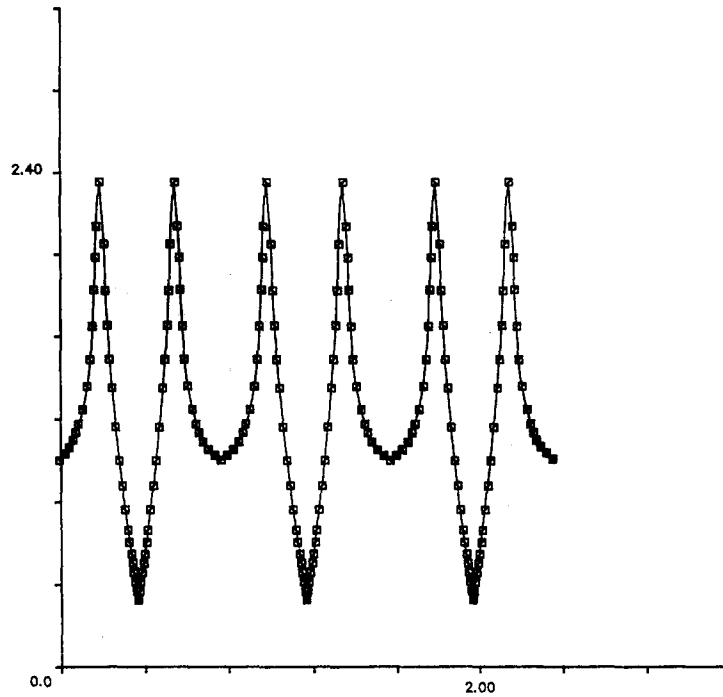


Figure 10.  $|u_{55}(x, t)|$ , computed along the direction of  $x = 0$  and for different values of  $t$  to show that of all spikes attain the same maximum value.

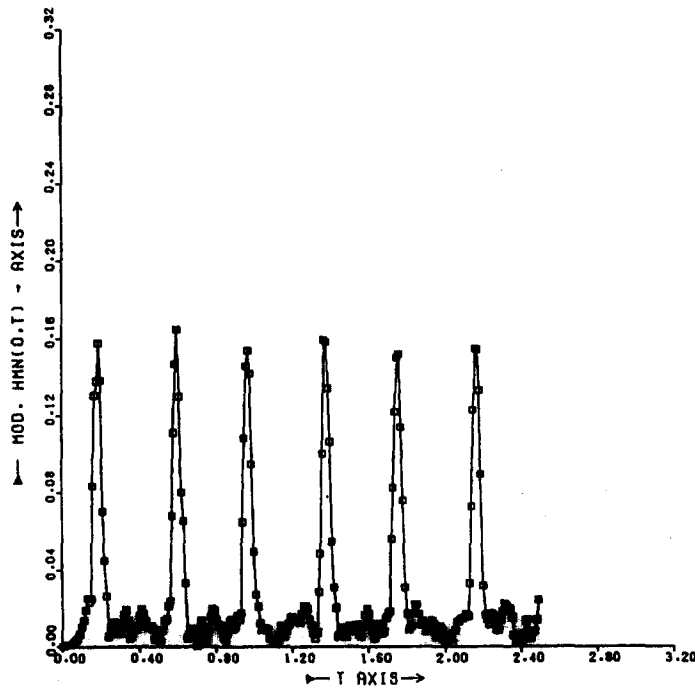


Figure 11. Behaviour of the modulus of the perturbation term  $|H_{55}(x, t)|$ , at  $x = 0$  and  $t \approx 0(0.01)2.5$ .

#### REFERENCES

1. M. Delfour, M. Fortin, and G. Payne, Finite-difference solutions for a non-linear Schrödinger equation, *J. Comp. Phys.* **44**, 277-288 (1981).
2. D.F. Griffiths, A.R. Mitchell and J.L.I. Morris, A numerical study of the nonlinear Schrödinger equation, *Comput. Math. Appl. Mech. Eng.* **45**, 177-215 (1984).

3. B.M. Herbst and A.R. Mitchell, The numerical stability of the nonlinear Schrödinger equation, Report NA/66, University of Dundee, (1983).
4. B.M. Herbst, J.L. Morris and A.R. Mitchell, Numerical experience with the nonlinear Schrödinger equation, *J. Comp. Phys.* **60**, 282-305 (1985).
5. J.M. Sanz-Serna and V.S. Manoranjan, A method for the integration in time of certain partial differential equations, *J. Comp. Phys.* **52**, 273-289 (1983).
6. J.M. Sanz-Serna, Methods for the numerical solution of the nonlinear Schrödinger equation, *Math. Comp.* **43**, 21-27 (1984).
7. J.G. Verwer and J.M. Sanz-Serna, Convergence of method of lines approximations to partial differential equations, Report NM-R8404, pp. 1-14, Centrum voor Wiskunde en Informatica, Amsterdam, (1984).
8. J.G. Verwer and J.M. Sanz-Serna, Conservative and non-conservative schemes for the solution of nonlinear Schrödinger equation, Report NM-R8405, Centrum voor Wiskunde en Informatica, Amsterdam, (1984).
9. C. Lanczos, Trigonometric interpolation of empirical and analytical functions, *J. Math. Phys.* **17**, 123-199 (1938).
10. E.L. Ortiz, The Tau Method, *SIAM J. Numer. Analysis* **6**, 480-491 (1969).
11. E.L. Ortiz, On the numerical solution of nonlinear and functional equations with the Tau Method, In *Numerical Treatment of Differential Equations in Applications*, (Edited by R. Ansorge and W. Törnig), pp. 127-139, Springer-Verlag, Berlin, (1978).
12. E.L. Ortiz and H. Samara, An operational approach to the Tau Method for the numerical solution of non-linear differential equations, *Computing* **31**, 95-103 (1983).
13. E.L. Ortiz and A. Pham Ngoc Dinh, On the convergence of the Tau Method for nonlinear differential equations of Riccati's type, *Nonlinear Analysis* **9**, 53-60 (1985).
14. P. Onumanyi and E.L. Ortiz, Numerical solution of stiff and singularly perturbed boundary value problems with a segmented-adaptive formulation of the Tau Method, *Math. Comput.* **43**, 189-203 (1984).
15. E.L. Ortiz and H. Samara, Numerical solution of partial differential equations with variable coefficients with an operational approach to the Tau Method, *Comp. and Math. with Applic.* **10** (1), 5-13 (1984).
16. E.L. Ortiz and K.S. Pun, Numerical solution of nonlinear partial differential equations with the Tau Method, *J. Comp. and Appl. Math.* **12-13**, 511-516 (1985).
17. E.L. Ortiz and A. Pham Ngoc Dinh, Linear recursive schemes associated with some nonlinear partial differential equations and their numerical solution with the Tau Method, *SIAM J. Math. Anal.* **18**, 452-464 (1987).
18. E.L. Ortiz and K.S. Pun, A bi-dimensional Tau-Elements Method for the numerical solution of nonlinear partial differential equations with an application to Burgers' equation, *Comp. and Math. with Applic.* **12B**, 1225-1240 (1986).
19. E.L. Ortiz, Step by step Tau Method: piecewise polynomial approximations, *Comp. and Math. with Applic.* **1** (3), 381-392 (1975).
20. R.F. Sincovec and N.K. Madsen, Software for nonlinear partial differential equations, *ACM TOMS* **1**, 222-260 (1975).
21. V.E. Zakharov and A.B. Shabat, Exact theory of two-dimensional self-focusing and one-dimensional self-modulation of waves in nonlinear media, *Sov. Phys. JEPT (English Trans.)* **34**, 62-69 (1972).
22. G.B. Whitham, *Linear and Nonlinear Waves*, Wiley-Interscience Series, New York, (1974).
23. R.K. Dodd, J.C. Eilbeck, J.D. Gibbon and H.C. Morris, *Solitons and Nonlinear Wave Equations*, Academic Press, London, (1982).
24. P.G. Drazin and R.S. Johnson, *Solitons: An Introduction*, Cambridge University Press, Cambridge, (1989).
25. C. Lanczos, Legendre vs. Chebyshev polynomials, *Topics in Numerical Analysis*, (Edited by J.J.H. Miller), pp. 191-201, Academic Press, New York, (1973).
26. E.L. Ortiz, Sur quelques nouvelles applications de la Méthode Tau, In *Seminaires IRIA*, (Edited by R. Glowinski and J.-L. Lions), pp. 247-257, IRIA, Paris, (1975).
27. S. Namasivayam and E.L. Ortiz, Dependence of the local truncation error on the choice of perturbation term in the step by step formulation of the Tau Method for systems of ordinary differential equations, In *Numerical Treatment of Differential Equations*, (Edited by K. Strehmel), pp. 113-121, Teubner, Leipzig, (1987).
28. A.R. Mitchell and J.L.I. Morris, A self-adaptive scheme for the nonlinear Schrödinger equation, *Arab Gulf J. Scient. Res.* **1**, 461-473 (1983).
29. A.B. Shamardan, The numerical treatment of Schrödinger equation, *Comp. and Math. with Applic.* **19**, 67-73 (1990).